

3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol
647-42-7 | DTXSID5044572

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.92e-03 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.21e-01

Confidence level: 5.07e-01

Nearest Neighbors from the Training Set

Image not found

1,1,1-Trifluoro-2-propanol

Measured: 2.04

Predicted: 2.45

Image not found

Fluopropanate-sodium

Measured: 1.31e-01

Predicted: 4.65e-01

Image not found

Cyclobutane, octafluoro-

Measured: 1.65e-04

Predicted: 1.51e-04

Image not found

Ethane, hexafluoro-

Measured: 5.64e-05

Predicted: 1.08e-04